On the Efficient Treatment of Data Covariance Matrices

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Modifications are proposed in the generation and treatment of off-diagonal data covariance matrices (DCM) for use in data-fitting: (1) Consistent and reliable results are obtained by defining the DCM in terms of the "true" value (not the measured value) of the quantity. An algebraic proof of this assertion will be presented. (2) For large numbers of data points, efficient and numerically stable results are obtained by writing the DCM in terms of its components and using matrix-manipulation techniques to avoid calculating, inverting, and storing large arrays. (3) Any parameter whose value and uncertainty are already known may be treated in two different ways: The parameter may be treated as a fitting parameter in the analysis; alternatively, the parameter's value may be held fixed and its uncertainty propagated through the data-fitting procedure. Results for all other parameters will be identical for the two methods. Details and examples for each of these proposals will be shown, based on their implementation in the SAMMY code[1] (which is used for analysis of cross-section data in the resonance region).

[1]"Updated Users' Guide for SAMMY: Multilevel R-Matrix Fits to Neutron Data Using Bayes' Equations," N. M. Larson, ORNL/TM-9179/R6, Oak Ridge National Laboratory, Oak Ridge, TN (May 2003).